2. BACKGROUND

This background chapter will review the key literature related to emissions modeling. Four general areas are reviewed: automobile exhaust emissions, emission rate modeling, motor vehicle activity modeling, and geographic information systems (GIS). The automobile exhaust emission section will focus on the cause and effect relationships of vehicle operation and emission production. The emission rate modeling section will focus on techniques used by different modeling approaches to determine vehicle emission rates. The vehicle activity section will review and identify techniques for developing estimates of emission-specific vehicle activity. The GIS section will discuss issues surrounding spatial and temporal modeling, and review past uses of GIS in the transportation and air quality arena.

2.1. Automobile Exhaust Emissions

This section discusses three topics that are important in motor vehicle exhaust emissions: the major pollutants, the cause and characteristics of their production, and the concept of modal emissions. Understanding these three is crucial to designing a system that is focused on cause and effect relationships.

2.1.1. Exhaust Emission Pollutants

The Clean Air Act of 1970 identified six air pollutants of concern in the United States: carbon monoxide (CO), hydrocarbons (HC), oxides of nitrogen (NOx), sulfur dioxide (SO_2), particulate matter (PM-10), and lead (Pb). Recently, PM-2.5 was added to this list. Nationally, in 1994, on-road vehicles were reported to contribute 62 percent of CO emissions, 42 percent of HC emissions, 32 percent of NOx emissions, ~5 percent of SO_2, 19 percent of PM-10 (PM-2.5 was unreported), and 28 percent of Pb [USEPA, 1995]. Carbon monoxide, hydrocarbons, and oxides of nitrogen are pollutants prevalent in automobile exhaust (PM-10 is produced by diesel engines and tire wear and Pb is being successfully reduced by its elimination from gasoline). For the purposes of this research, the term 'emissions' will hereafter refer to CO, HC, and NOx. All of the pollutants present health dangers to people, animals, and vegetation. Ozone (O_3) is produced through a complex series of chemical reactions that result from pollutants (HC and NOx) mixing in the atmosphere in the presence of sunlight. Generally, ozone concentrations are highest in urban centers and downwind of urban centers. Ozone has been observed to vary spatially in an urban area, and that the production of ozone is the result of pollutants mixing in space and time. It is also interesting to note that biogenic sources of HC contribute significantly to ozone production. For example, in the southeast United States, eliminating all the anthropogenic (man-made) sources of HC would still not result in passing federally mandated ozone standards due to the levels of HC produced by biogenic (vegetation) sources. [SOS, 1994]. This indicates that a NOx reduction policy would better serve ozone reduction in the southeast [NRC, 1991].

On-road vehicles have been significant contributors to air pollution since the 1940s. The trends in new car emission rates of CO have shown significant improvement over the last thirty years. The improvements have been attributed to legislatively induced emission controls for new vehicles (see section 2.1.2). The actual transportation contribution to overall CO emissions, however, has not declined at the same rate, due in part to the fact that the mobile emission controls are designed to affect only a portion of the engine operating mode and because per capita vehicle miles of travel have increased. In fact, vehicle miles of travel (VMT), auto ownership, person trips, and fraction of single occupant vehicles (SOV) have increased disproportionally to population growth [Johnson, 1993, Meyer, 1997].

2.1.2. The Mechanics of Exhaust Emissions

In ideal combustion, oxygen and fuel (HC) are combusted and produce byproduct emissions of carbon dioxide (CO_2) and water (H_2O). Air, however, contains nitrogen (N_2) among other chemicals, and combustion is always incomplete, producing byproducts of HC, CO, oxygen (O_2), carbon dioxide (CO_2), water (H_2O), and NOx [Heywood, 1988, Jacobs, 1990]. The air to fuel (a/f) ratio is an important factor in determining the quantity of pollutants produced by combustion. Generally, rich fuel mixtures (low a/f ratios) produce high amounts of CO and HC because combustion is incomplete. Lean fuel mixtures (high a/f ratios) will typically produce higher amounts of NOx (especially during very hot, lean conditions) and lower amounts of CO and HC because combustion is more complete. When considering vehicle activity, high power demand (sharp accelerations, heavy loads, etc.) creates a rich fuel mixture resulting in elevated CO and HC emission rates while NOx generally decreases. At high speeds with low acceleration rates, a lean fuel mixture develops which increases NOx emission rates [Heywood, 1988].

Car manufacturers design automobile engines to maximize fuel efficiency and to comply with federal certification tests (Federal Test Procedure (FTP)), which means balancing the a/f ratio (through computerized engine controls) to its most efficient point (stoichiometry). However, car manufacturers also design automobile engines to provide power to meet consumer demand. The certification tests do not cover the high speeds (maximum speed is 56.7 mph) and high accelerations (maximum acceleration is 3.3 mph^2/sec.) where rich and lean mixtures occur [Barth, 1996]. Therefore, all automobiles are allowed to have inefficient combustion at the high ends of the speed / acceleration spectrum in order to provide drivers with greater power on demand. New test cycles would provide incentives for car manufacturers to reduce the designed enrichment events resulting from power demand. This reduction could significantly lower new car emission rates.

Vehicle technology has changed dramatically over the last thirty years and great strides have been made in reducing emissions. In the 1960s, many vehicles were fitted with devices that controlled the amount of fuel used for combustion, thereby improving the efficiency of combustion and reducing exhaust emissions. In the late 1970s and early 1980s, catalytic converters were installed on new vehicles. Initially, these catalytic converters focused on controlling CO and HC emissions. The catalytic converters treated exhaust gas by removing much of the CO, HC, and NOx emissions [CARB, 1990]. Because there is variability over time (model year) in the types of emission control devices installed on new vehicles, it is probable that vehicle characteristics will play an important role in predicting emission rates, and thus be an important feature in model design for many years to come.

Because emission control technology significantly impacts emissions generation, there are large differences between vehicles with functional control systems, and those with malfunctioning, deteriorated, or nonexistent control systems. The latter group can have significantly higher emissions [Pollack, 1992]. The differences can be pronounced enough that researchers have termed the high emitting vehicles ‘high emitters.’ Correct representation of high emitters in the vehicle fleet will be crucial to accurate emission modeling efforts given the magnitude of these “above normal” emissions.

2.1.3. Modal Emissions

Modal emissions refers to the types of emissions related to specific modes of operation. Figure 2.1 conceptually represents the relative magnitudes of exhaust emissions for a vehicle trip in space and time. As seen in the diagram, the initial rate of emissions is high, indicating engine start mode. After the engine warms over a period of time, emissions drop and stabilize (hot-stabilized mode). The stabilized rate is interrupted by periods of high emissions (enrichment mode). Each of these three automobile exhaust-operating modes is discussed in the following sections.

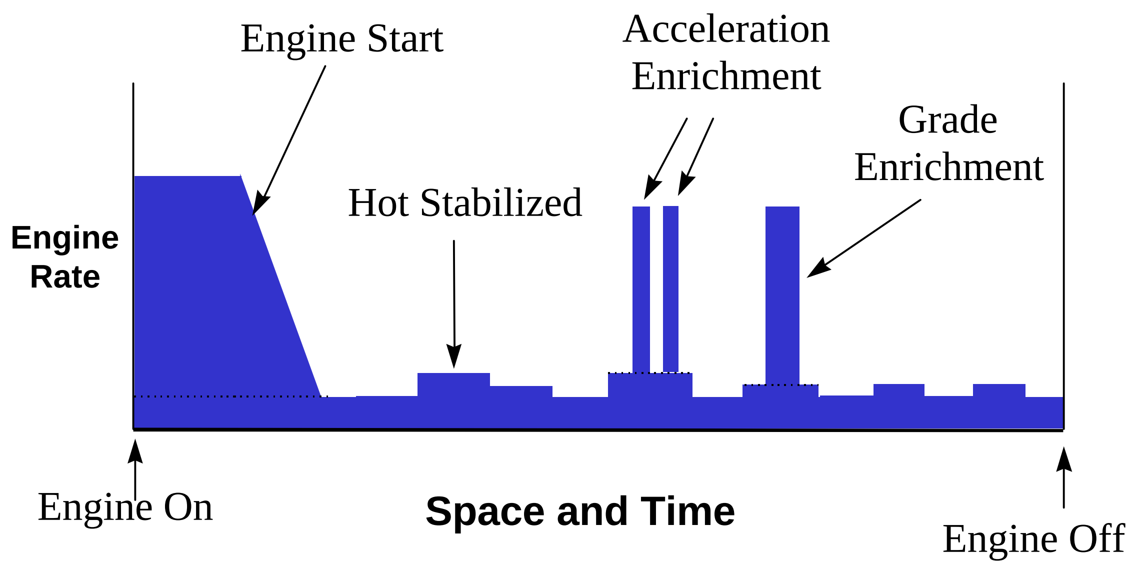

Figure 2.1 - CO Emissions for a Hypothetical Vehicle Trip

2.1.3.1. Emissions in Start Mode

Motor vehicle emission rates are elevated during the first few minutes of vehicle operation. This is primarily caused by emission control equipment that functions well only at high temperatures. The magnitude of the emissions is a function of: commanded air/fuel ratios, catalyst temperature, and engine temperature (Jacobs, et al., 1990; Heywood, 1988; Joy, 1992; Pozniak, 1980). Most onboard computer control systems initially demand an enriched fuel mixture so the engine will not stall or hesitate during the warm-up period. Thus, the high emissions concentration in the exhaust plume is initially a direct function of the computer control system which varies from vehicle to vehicle. Commanded enrichment may cease when a specific time has passed or when a specific coolant temperature is reached. As engine temperatures rise, combustion efficiency improves and emissions concentrations are gradually reduced. Finally, to be effective, catalytic converters must reach "light-off" temperatures of roughly 300 ^{o}C. Until the catalyst reaches this temperature, emission concentrations in the exhaust plume remain high. Catalyst temperature rise is a function of initial catalyst temperature, exhaust gas temperatures, exhaust gas volumes passed through the converter, and emission concentrations. Thus, the magnitude of elevated emissions associated with engine starts is also a function of the amount of time the vehicle has remained inactive (that affects the catalyst and exhaust gas temperatures), and a function of the manner in which the vehicle is operated after the engine is started (which affects exhaust gas volumes and hydrocarbon loading). Cold starts, engine starts that occur when the engine temperature is below the catalyst light-off threshold, have higher CO and HC emissions.

Two approaches have typically been employed to model engine start emissions: 1) starts are modeled as discrete emission-producing activity, or a “puff,” and 2) starts are modeled as a function of a base emission rate (hot-stabilized exhaust) adjusted for conditions that elevate emission rates (Guensler, 1994). The California Air Resources Board's (CARB's) emission rate model (EMFAC7F), for example, treats the elevated engine start emissions as a single "puff" (i.e. separate from running exhaust) and multiplies the number of engine starts by a cold start emission rate. The US Environmental Protection Agency's emission rate model (MOBILE5a), on the other hand, increases the calculated running exhaust emission rate for vehicles, based upon an assumed fraction of vehicles operating in cold start, hot start, and hot stabilized modes. MOBILE5a documentation recommends using 20.6% as the percentage of operating vehicles in cold start mode and 27.3% in hot start mode (based on the FTP analysis). These percentages do not consider location or functional class and were highly correlated to time of day and trip purpose [Venigalla, 1995a].

Historically, the number and location of cold starts have been based on trip generation models (see section 2.3.1) using socioeconomic predictors. Considering emission output, the major factor is not the actual number of starts, but the duration and location of a vehicle operating in start mode. Therefore, a vehicle trip lasting through the start mode will have significantly greater total pollutant production than the few seconds of a false start (an engine start that does not result in a vehicle trip). Research has shown that 180-240 seconds is the approximate average cold start mode duration. In 200 seconds, a vehicle traveling at 35 mph can travel over two miles. A spatially resolved model of start emissions must be able to identify the trip origin and the point on a traveled route where a vehicle moves from elevated emissions in start mode to reduced emissions in hot-stabilized mode. Given that the actual duration of the start mode is not necessarily 200 seconds but a function of a number of engine parameters and conditions, the ability to model on a large scale where the switch in operating modes occurs for a fleet of operating vehicles becomes quite complex. Because trip generation is estimated on a zonal basis, a zonal distribution of engine parameters and conditions may provide enough regional disaggregation and zonal aggregation to identify quantities of pollutants produced. Crucial to success, however, is the size of the zone.

The determination of whether a start is “cold” or “warm” (a warm start occurs when the engine is still warm and therefore closer to catalyst light-off temperature) is also a difficult problem. The duration of the engine soak time (length of time the vehicle is not running) has been used to determine whether a vehicle has a cold or warm engine, thus affecting the duration of elevated emission rates [Sabate, 1994]. Cold starts occur after 4 hours of engine-off activity for non-catalytic converter vehicles, and after 1 hour for catalyst equipped vehicles. Therefore, the parking duration of vehicles indicates how long it will take before the engines warms sufficiently after a start.

The engine “cold” and “warm” start conditions pose a difficult modeling problem. The temporal characteristics of vehicle start activity play an important role in predicting appropriate emission rates. The travel patterns of vehicles also become important. A model including cold and warm start vehicle activity must be spatially and temporally resolved and include predictions of travel behavior and vehicle technology descriptions.

2.1.3.2. Emissions in Hot-stabilized Mode

Hot-stabilized emissions occur after a vehicle’s engine has reached sufficient catalyst light-off temperature. When the emission control equipment runs efficiently, emission rates reach a low, fairly stable level. The stabilizing effect also occurs on non-catalyst vehicles due to decreased commanded enrichment, cylinder quenching, and engine oil viscosity. The stabilized emission rates actually fluctuate slightly according to vehicle characteristics, environmental conditions, and vehicle operating modes [Guensler, 1993a]. Vehicle characteristics that have been identified as possibly having explanatory power for a vehicle’s emission rate include model year, engine size, accrued mileage, emission control equipment type (such as catalytic converter type) and condition, fuel delivery technology, engine monitoring and control strategies (integrated into the electronic control module), gear shift ratios, and vehicle weight and shape (for aerodynamic drag) [Guensler, 1994, Barth, 1996]. Environmental conditions include ambient temperature, altitude, and humidity [Guensler, 1994, Barth, 1996]. Vehicle operating modes include cruise, acceleration, deceleration, idle, and induced vehicle loads (e.g., number of passengers, trailer towing, grade, and air conditioning) [Guensler, 1994, Barth, 1996]. A vehicle can move in and out of hot-stabilized emission mode when sufficient power is demanded causing a rich air to fuel ratio. When power is demanded causing an enriched fuel condition, emission rates change dramatically (see section 2.1.3.3).

Current models account for some but not all of the factors listed above. Instead, surrogate factors, which are correlated to the factors of interest, are used because they are much easier to obtain for a regional fleet of vehicles. For example, in the EPA MOBILE5a model and the California Air Resources Board EMFAC7F models, the effects of acceleration, deceleration, cruise and idle are currently represented by a single surrogate factor, average operating speed. Average operating speed is correlated with different proportions of vehicle operating modes. Surrogate vehicle attributes include model year, fuel delivery technology, catalytic converter type, accrued mileage, and vehicle condition, and are relatively easy to obtain or estimate for a regional fleet of vehicles from registration and inspection / maintenance databases .

2.1.3.3. Off-Cycle Exhaust Emissions

Off-cycle emissions are those emission events which occur outside the envelope of the Federal Test Procedure (FTP). The FTP dynamometer test cycle was used as the basis for current model emission rates. Because the FTP cycle did not include vehicle activity with speeds above 57 mph and accelerations greater than 3.3 mph/sec, a certain portion of actual vehicle activity is unrepresented in the test dataset. Activity outside the tested ranges would represent high engine loads and throttle positions that push engines into enrichment conditions. These events are of crucial importance, not just because they aren't included in the analysis of emission rates used for current models, but because these events are known to produce the highest emission rates [Benson, 1989; Groblicki, 1990; Calspan Corp., 1973; Kunselman, et al., 1974]. In fact, one sharp acceleration may cause as much pollution as does the entire remaining trip [Carlock, 1993]. Emissions models may be underpredicting emissions by fairly high margin.

Spatial modeling of off-cycle exhaust emissions requires the ability to predict vehicle speeds and accelerations at a resolution deemed significant by emission rate research. Speeds and accelerations could identify the fraction of the fleet that may be unrepresented in current emission rates. Further, research into the reanalysis of second by second emission test data is discovering substantial amounts of test data outside the FTP envelope [Siwek, 1997]. The reanalysis could predict emission rates based on speed and acceleration characteristics. Further, there is a need to develop emission estimates at a facility level [Venigalla et al.,1995a]. That is, it must be able to predict the locations of enrichment events. If facility-level speed and acceleration profiles can be predicted, emission rates can be applied.

2.2. Automobile Exhaust Emission Rate Prediction

Three emission rate modeling approaches are discussed in this section; an emission-factor approach, a physical approach, and a statistical approach. Each model type has particular advantages and disadvantages. All of the approaches suffer from two limiting factors:

Inadequate Vehicle Test Data. There is a significant amount of emission test data compiled over the years (over 700 vehicles and over 8000 vehicle tests). Most of the testing was done by agencies attempting to determine new car conformity to emission standards. New cars are run through the Federal Test Procedure (FTP) which is a set of three test cycles run on a dynamometer. There is a cold start cycle (bag 1), a running exhaust cycle (bag 2) and a hot start cycle (bag 3). The cycles are called 'bag' data because emissions are collected in a bag during the test. All of the test datasets suffer from at least one of two major limitations, sample size and (or) unrepresentative cycles. The FTP cycle, for example, does not test accelerations above 3.3 mph/sec or speeds above 57.5 mph. Other test cycles that have high speed and acceleration data do not have a representative sample of the on-road fleet.

Inadequate prediction of emission-specific vehicle activity. Emission-specific vehicle activity refers to the division of vehicle operation into groups that differ significantly in their resulting emission rates. All of the approaches require vehicle activity as an input. The best predictor of vehicle activity for metropolitan areas is currently the four-step Urban Transportation Planning System (UTPS) (see section 2.3.1). Although advances have improved the ability of these models to predict emission-specific vehicle activity, most MPOs still use models that have significant errors in facility-level estimates of volume and average speed [Stopher, 1993, Harvey, 1991, Outwater, 1994].

All of the modeling approaches focus on developing emission production estimates, but few present systems are designed to address facility-specific impact issues. This issue is crucial in defining which emission rate model approach best fits the technical capabilities and economic constraints of agencies required to make estimates. In other words, the most accurate model for predicting the emissions of an individual vehicle may not be the most useful for certain types of modeling situations. It may also become evident that the understanding of the causes of an individual vehicle's emission rate has greatly surpassed the ability to collect the input variables for a real-world operating fleet. Important to this issue is the level of aggregation manifested in deterministic or stochastic approaches.

2.2.1. A Speed Correction Factor Approach

Both the USEPA's and the CARB's modeling systems use a 'speed-correction factor' approach to predict aggregate emission rates. The systems are mandated for use in conformity determination despite their widespread statistical and theoretical criticism. The models select a base emission rate depending on a variety of vehicle technology and environmental parameters. The base emission rate is then factored or adjusted based on the ratio of the observed speed to the average FTP cycle bag 2 speed (16 mph). As the models are currently used, the documentation suggests using default values for national fleet averages and other variables. On the positive side, the modeling system is not data intensive, it requires only inputs of total vehicle miles traveled (VMT), average speed, and a cursory knowledge of fuel type and climate data to get estimates of pollutant production. The system is easy to use and widely implemented by agencies without significant capital or operating expense. On the negative side, it is not responsive to changes in important variables (acceleration, fleet makeup, engine load, etc.).

The emission rate models are based on data collected from the FTP cycles developed for new car emission testing. Added to the problems noted earlier with the FTP cycle data, the modeling methodology is highly aggregate and therefore insensitive to microscale variability [Guensler et al., 1993b]. The approach, therefore, may not be able to accurately identify the best choice between small scale development alternatives (changes in lane widths, signal coordination, etc.).

The EPA's Office of Mobile Sources continues to support research which will help to identify incremental improvements to their modeling process. Currently, MOBILE 5a is the mandated emission rate model, and MOBILE 6 is under development. Modal issues, non-FTP cycle estimates, and other emission rate specific factors are planned for implementation.

2.2.2. A Physical Approach

The physical or deterministic approach to emissions modeling is designed to develop accurate emission estimates using many variables. The University of California at Riverside is currently developing such a modal modeling approach under a three year National Cooperative Highway Research Program project. The approach will track the vehicle components and conditions that affect emission rates. The model is designed to track an individual vehicle's power demand and engine equipment status. Power demand is predicted using environmental parameters (wind resistance, road grade, air density, temperature, and altitude), and vehicle parameters (velocity, acceleration, vehicle mass, cross-sectional area, aerodynamics, vehicle accessory load, transmission efficiency, and drive-train efficiency). Power demand is combined with other engine parameters (gear selection, air/fuel ratio, emission control equipment, and temperature) to develop dynamic vehicle or technology group emission rates. When combined with a vehicle's operating parameters, deterioration (the change in emission rate over time due to catalyst decay or equipment malfunction), and fuel type, the model produces highly time resolved emission estimates which promise to be more accurate at the microscale level than any model produced thus far. Vehicle test data for their model are being collected on dynamometers (~300 vehicles) as part of the project. Final test data should be available in two to three years [Barth 1996].

Barth, et al. recognize that their approach is data intensive, but accurate emissions modeling forces it to be so. The vehicle data requirements are many and go beyond the availability of information found in vehicle identification numbers (VINs) that are maintained by state registration datasets. A lookup table could be developed for missing parameters based on vehicle make, model, and model year. Other data (environmental, and operating conditions) would have to be developed from other models. The physical approach fits well with a simulation model of vehicle activity (see section 2.3.2) because the simulations track individual vehicles.

The use of the physical model approach for regional impact modeling requires data aggregation. As with other models, the approach is plagued by poor estimates of emission-specific vehicle activity. Because the physical approach appears to be the most accurate model for predicting an individual vehicle's second-by-second emission rate, vehicle-specific second-by-second activities are needed to get accurate results. Because accurate prediction of these parameters relies on predicting human behavior among other highly variable data, it is likely the activity estimates will have high variability. Aggregating to statistical distributions of the data will lessen this problem, but departs from the original intention of highly accurate second-by-second estimates. The large number of input variables introduce error associated with the ability in predicting their values. The algorithms may be solid, but data input error could significantly degrade the accuracy of the final estimate.

2.2.3. A Statistical Approach

Researchers at Georgia Tech have developed a modeling approach that is based on statistical distributions of a variety of vehicle technologies and vehicle operating modes. The core of the emission rate model is based on hierarchical tree-based regression analysis (HTBR). The tree analysis is a statistical procedure that iteratively splits a dataset into two parts by; (1) selecting a variable that controls the most variability, and (2) determining a cutpoint of that variable that explains the most variability. The result is a 'tree' where each ending node is a set of predictor variable conditions, and an emission rate (for each pollutant and operating mode). Once a 'tree' is developed, adjustments are made to the values based on load (from wind resistance, grade, and accessories).

Georgia Tech researchers combined a variety of emission test datasets from a number of sources in order to maximize the comprehensiveness of the vehicle fleet and potential operating conditions. The data have been re-analyzed to allow modal parameters to be included. Although there are still limitations with the dataset (representative fleet and cycle operating conditions), an extensive emission rate 'tree' has been developed. The HTBR approach is also plagued with the lack of availability of adequate data input. Extensive vehicle data (model year, engine size, fuel system, emission control, vehicle class, vehicle test weight) and vehicle operating data (speed, acceleration) are needed for predicting emissions. One benefit to the approach is that it can be adjusted for missing data. If one particular variable is missing from the dataset (vehicle test weight, for example, is not stored in the Vehicle Identification Number), the HTBR can be re-run and produce new emission rates that exclude that variable. The new rate may, however, be less accurate, depending on how significant the missing variable is to emission estimation. Another benefit to the statistical approach over current models is the ability to put confidence bounds around each estimate. This becomes important when estimates for a variety of conditions on a certain facility segment are added together to produce a single facility estimate, whose accuracy must be quantified.

Critics of this modeling approach have suggested that the inability to track causal variables results in a model that is unable to predict the effects of new technology. There are three counter-arguments to this criticism, (1) because control standards continue to tighten, it is more important to model the old technology instead of the new, (2) no model can expect to accurately predict future technology changes, they can only develop relationships based on known conditions, and (3) if surrogate variables are correlated to casual ones, the model will still continue to work.

2.2.4. Emission Rate Modeling Summary

The microscopic physical approach taken by Barth et al. has the potential to provide the most explanatory power, disregarding input data error issues that can't be quantified at this time. It is also clear from the research that the speed correction factor approach is highly aggregate and inappropriate for the modeling needs of research and planning agencies. The statistical approach provides near-term improvements and allows for facility level aggregations of data. An important factor in selecting a particular emission rate modeling approach is its ability to fit within the framework of the larger 'data model' issues regarding the user needs of measuring and predicting transportation impacts on air quality. The 'data model' in this context refers to the design of an entire modeling system from user needs to data structure and connectivity. The statistical approach seems most appropriate given the scope of this research because it appears to fit the balance between accuracy and implementability identified as a modeling objective in Chapter 1.

2.3. Vehicle Activity Modeling

2.3.1. Urban Transportation Planning System (UTPS)

The Urban Transportation Planning System, (or travel demand forecasting model), first developed in the 1960s, was designed to predict travel flows within an urban area. The primary purpose of the system was to guide new infrastructure investment [Outwater, 1994]. Because of its predictive nature and widespread use, the use of this modeling approach has expanded beyond the original intent to predicting emission-specific vehicle activity. Until recently, vehicle activity has meant vehicle miles traveled (VMT) and average speed, the inputs to mandated emission models. However, as understanding of emission behavior expands, so does the definition of vehicle activity. Emission-specific vehicle activity now encompasses detailed modal parameters which UTPS models are incapable of predicting. Researchers have identified numerous deficiencies in the approach (outside implementation problems); the facility level (link) estimates are highly variable, the models do not predict off-peak travel well, seasonal variations in travel are not considered, model size is limited, and the models are not sensitive enough to measure mandated TCM effectiveness [Stopher, 1993, Harvey, 1991, Outwater, 1994].

Along with theoretical problems, there have been a significant number of implementation problems including: lack of feedback components, insufficient current socioeconomic data and inadequate validation procedures [Harvey, 1991, Outwater, 1994]. Model results have indicated an accuracy range of 5-30% error in overall VMT estimates and 5-20 mph error in average speeds. [Miller, 1995]. Average error by models implemented by MPOs is 10% for VMT and 15 mph for average speed [Stopher, 1993]. Errors also increase as one moves from higher to lower road classifications. To add to the problems, the same models that are criticized as too simplistic are too complicated and costly for proper implementation by many agencies.

Despite these errors and theoretical deficiencies, the models represent the state-of-the-practice. In fact, they represent the only short and medium range alternative available for widespread implementation. There is a significant amount of research on techniques for improving the UTPS and hopefully improvements will result in better predictions of vehicle activity in time and space.

The Travel Model Improvement Program administered by the US Department of Transportation is attempting to improve the travel forecasting capabilities. Some of the potential improvements to predicting emission-specific vehicle activity are as follows. (1) There is a shift away from trip-based models towards activity-based models. Activity-based models better represent temporal changes and mode alternatives. (2) Development of stochastic microsimulation techniques aggregated to area traffic patterns will allow improved sensitivity to temporal changes. (3) The use of longitudinal panel surveys will more accurately identify cross-sectional survey (current technique) biases.

2.3.2. Simulation Models (TRANSIMS)

Simulation models are being viewed by many as the solution to the problems facing the UTPS. Simulation models generally come in three forms, microscopic, mesoscopic, and macroscopic. Microscopic models track individual vehicles and their relationships with other vehicles. Macroscopic models approximate traffic flow as a fluid and use a facility (road segment) as a the base unit. Mesoscopic models combine elements of both depending on the needed function. Simulation models have successfully been used for optimization (signal timing, traffic flow) and for forecasting (predicting results of a change). Models can be deterministic or stochastic (by allowing some randomness into the process). By their nature, simulation models have the theoretical and computational capability to predict facility-level activity at a resolution needed to predict emission-specific activity. The structure and data requirements of existing models have prevented their implementation for an entire urban structure, and force use at the facility level. Most models have been developed to answer specific problems instead of complete system simulation. However, a new generation of simulation models is taking a broader scope and the models are being designed around regional systems instead of specific traffic-flow issues. Recent advances in modeling theory, microscopic modeling, and computing power may have expanded the role of traffic micro-simulation modeling from the facility scale to the urban/regional scale.

Advances made by “TRANSIMS” (Transportation Analysis and SIMulation System) have led many to believe that they have found a replacement for the UTPS type models. TRANSIMS is being developed under the US Department of Transportation’s Travel Model Improvement Program and funded by the Federal Highway Administration and other federal agencies. The intent of the project is to develop a system that will be able to answer questions regarding policy and infrastructure change for an entire urban area. One of their major selling points is their focus on predicting air quality and other environmental impacts.

TRANSIMS will be a set of modules that can be run separately or together. The first module is a household and commercial activity module that uses US Census data to develop a synthetic population of individuals for Census Tracts and Block Groups and predicts synthetic economic activity and resulting travel demand. The second module is the intermodal route planner that takes the activity-based travel demand and develops trip plans for every individual that can be adjusted depending on the activities of other individuals over time. The third module is the travel microsimulation module that tracks individuals and their vehicles, and their relationships to other vehicle activities, on the road network using a ‘cellular automata’ technique. The final module is the environmental module that predicts a variety of environmental conditions including mobile source emission prediction, atmospheric mixing, and concentrations. The outputs of TRANSIMS will be summaries of second by second data at cells of 7.5 meters.

TRANSIMS promises to provide unique solutions to the integration of macroscopic and microscopic transportation modeling and provide advances in a number of simulation issues. Issues that the developers must address are validation and implementation. All of the new algorithms and techniques must be individually validated against observed data. The time frame and cost of implementation at a new urban area may be extensive due to the input data requirements.

Despite a number of issues that must be addressed by TRANSIMS developers, it is apparent that the spatial and temporal resolution of emission-specific vehicle activity could be substantially improved by TRANSIMS in the future. This aspect identifies the emission modeling need for incremental research that builds towards a future system that can move toward the objectives defined by the Los Alamos researchers.

2.4. Geographic Information Systems

A geographic information system (GIS) is “a computer-based information system that enables capture, modeling, manipulation, retrieval, analysis and presentation of geographically referenced data” [Worboys, 1995]. The rise of GIS technology and its use in a wide range of disciplines provides transportation and air quality modelers with a powerful tool for developing new analysis capability. The organization of data by location allows data from a variety of sources to be easily combined in a uniform framework. For example, vehicle registration information can be combined with census data to develop driver-vehicle profiles. Or, high traffic volume areas can be combined with satellite analysis of vegetation decay to study environmental impacts. Another important feature of GIS is its ability to bridge the technical gap between analysts’ and decision-makers’ need for easy-to-understand information . The communication power of GIS (thematic maps, GUIs, 3-D surface plots, etc.) is a feature that has made GIS one of the most used platforms for planning in the U.S. GIS provides the ability to get quick answers to technical questions. Literature on GIS data structures, applications, and vendor products is substantial. The following section will briefly cover, 1) the extent of GIS implementation by transportation and air quality agencies, and the past use of GIS in transportation and air quality analysis, and 2) the issue of spatial data quality.

2.4.1. GIS in the Transportation / Air Quality Agencies

The National Cooperative Highway Research Program (NCHRP) *Report 359* studied GIS in an effort to define its potential for transportation agencies. The document, which presented a comprehensive overview of GIS technology, its potential role for serving the needs of a variety of agencies, and strategies for successful implementation, stated,

> " The potential impact of GIS-T is profound. If this technology is exploited to its fullest, it will become ubiquitous throughout all transportation agencies and will become an integral part of their everyday information processing environments. … The potential impact of GIS is more than just agency wide. The problems of today require the interaction of agencies at all levels of government. … the broad problems that are driving the interaction typically involve environmental and economic development issues; and their solutions will require the integration and analysis of geographically referenced data of many kinds from many sources."

2.4.2. Applications of GIS in Mobile Emission Modeling

2.4.2.1. Emission Inventories

Bruckman et al. presented a paper in 1991 at an Air and Waste Management Association conference describing the use of GIS in developing gridded, hourly estimates of emissions. They also developed a model called CAL-MoVEM that utilized GIS in developing mobile source estimates for input into photochemical models. The main function of the GIS in their model was the spatial aggregation of travel demand forecasting model features into a grid. They used spatially defined vehicle mixes by trip purpose, temporal factors, hourly temperatures, trip volumes, trip speeds, and modal percentages as inputs. The spatially defined inputs were combined with EMFAC7E emission rates to produce gridded hourly estimates of pollutants [Bruckman, 1991]. The work was accomplished as part of a study on ozone levels in the San Joaquin Valley in California. Zonal estimates were allocated to TAZ (traffic analysis zone) centroids that were re-allocated to grid cells. Link estimates were allocated to nodes and re-allocated to cells. The use of points to represent these features did not take full advantage of the spatial structure provided by the original input data. TAZs falling along grid cell boundaries should have their portions divided. This strategy would limit grid cell sizes to those significantly larger than TAZs, which can be quite large (30-40 square km) for some metropolitan areas. Also, no mention is was made of strategies for identifying the confidence ranges of the estimates.

The model supports the use of GIS, but did not take full advantage of the research value of GIS. Further, the model did not have the flexibility to answer the diverse impact or mitigation questions that arise from estimating emissions.

2.4.2.2. GIS for Transportation Planning and Air Quality Analysis

Researchers used GIS as a preprocessor and postprocessor to mobile emission modeling. Although they relied on existing models to estimate emissions, they showed how GIS could be valuable in the management of emission related data. They made the connection between the needs of transportation planners and decision-makers and the spatial tools and features of GIS [Souleyrette 1991].

2.4.2.3. Microscale Analysis

Researchers at Utah State University used GIS in developing microscale analyses of a small group of intersections. They linked a GIS with CALINE3 and CAL3QHC to predict pollutant concentration levels [Hallmark, 1996]. The value of GIS (outside of spatial data storage and data visualization) was its ability to compare concentration results to other non-related data. The contribution is significant to this research because it provides a foundation for the argument that a GIS approach is not restricted to developing emission inventories, but can be easily expanded to a number of other related issues.

2.4.2.4. Influencing Decision-makers

Othofer et al. developed an interesting approach to predicting location specific emission production estimates for changing control strategies. Instead of developing estimates using detailed location-specific emission producing activities and emission rates, they disaggregated large zonal estimates using emission-producing activities [Orthofer, 1995]. The advantage of this approach is its simplicity and its straightforward recognition that the data needed to predict emissions at smaller levels does not exist or the relationships are undefined. The disadvantage is that the ability to predict changes among the disaggregated levels is a function only of the change of the overall larger units. Thus, the true effects of activity changes on emissions cannot be measured. The project produced high-quality graphics that indicated locational variation in emission-producing activities. The project was successful because elected officials could ‘see’ areas that have potentially high emissions and therefore had evidence for developing actions for those specific areas. Although, the modeling capability of the project is limited, its ability to influence action through spatial communication is a noteworthy contribution to the use of GIS in this arena.

2.4.3. Spatial Data Issues

Spatial data refers to points, lines, or polygons that maintain a digital connectivity with other entities in regards to their relative position. Spatial data comes in two forms, raster or vector. Raster data is information in a regular unit, usually a grid cell. The grid cell maintains an attribute value and locational information pertaining to its place in a matrix. Raster data is preferred when representing continuous data (natural features, environmental features, air quality, etc.) or when developing complex spatial data models. Vector data is information in the form of points, lines, or polygons. Vector data better represents features with discrete edges (anthropogenic features, rivers, transportation, etc.). An issue of prime importance to both data structures, and for this research, is spatial data quality. The quality refers to a number of issues regarding the accuracy and resolution which are discussed in the next two sections.

2.4.3.1. Positional Accuracy

Positional accuracy refers to the variability of the represented position from the actual position. Relative positional accuracy refers to the relational position between represented features and absolute position accuracy refers to the relationship between represented features and the Earth's surface. A good relative accuracy and poor absolute accuracy indicate a positional problem that is important when bringing different databases together. Because of the development of US National Map Accuracy Standards and the advent of improved surveying techniques, relative positional accuracy within a single dataset is not significant given the scope of inventory modeling. Absolute positional accuracy becomes an issue when joining multiple spatial databases. Variations in position can result from using different projections, datums, or transformations. Any attempt to join spatial databases must address the issue and provide solutions (stretching, fuzzy tolerance, etc.) to reduce the impacts.

2.4.3.2. Data Resolution

Data resolution concerns the level of spatial aggregation, or density of observed values. Data resolution usually refers to the scale at which the original data observations were made, and the level of interpolation used in developing the final dataset. The level of resolution is important in determining the confidence of a represented value at a particular coordinate. As in positional accuracy, data resolution problems usually occur when trying to combine databases of varying resolution. The combination of two datasets will result in a dataset that has a resolution equivalent to the one with less detail. This is frequently overlooked in analysis resulting in the presentation of data with significant variance. For example, soils data at a scale of

1:24,000 can be overlaid with 1:100 parcel data in an attempt to identify the parcel's soil type. The result represents the 'best guess' as to soil type variations within a parcel, but the variability is high. It is good practice to question whether the scale of database fits the spatial character of what is being represented. For example, does a 1 km or 4 km aggregation of ozone precursor pollutants provide enough resolution given the scale of ozone formation?

2.4.3.3. Data Content Accuracy

Data content accuracy refers to the accuracy of the attribute data represented by the spatial feature. Data content accuracy can be limited by a number of procedural problems (coding error, measurement error, etc.) or by the change of the data over time. Data content can be estimated by validation techniques, but they are usually cost-prohibitive for the large spatial datasets available. Usually spatial databases can be tracked to an original collection technique that may have been validated. It is also possible to compare two or more datasets for agreement to develop a qualitative appraisal. Most publicly available datasets have quantitative information on the accuracy of their data content.